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INTEGRAL DIFFUSION PROBLEMS

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Section I. Solution of the Equation

Classified according to the Atomic Energy Commission by authority of the U.S. Atomic Energy Commission

Per H.F. Carroll, 3-2-56, List No. 3

A. Equations.

The diffusion, multiplication, and ~~absorption~~ <sup>absorption</sup> of neutrons may be

described by the integral equation:

$$\rho(\vec{r}, t, \vec{v}) = \int d\vec{v}' \int_0^{s_m} ds \sigma(\vec{v}, \vec{v}') e^{-\Sigma(\vec{v})s} \rho(\vec{r}-s\vec{v}/|\vec{v}|, t-s/|\vec{v}|, \vec{v}') \quad (1)$$

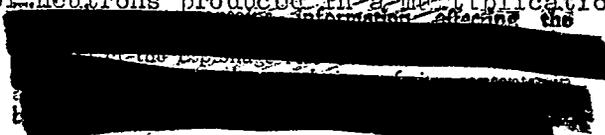
where  $\rho(\vec{r}, t, \vec{v})$  is the density of neutrons at time  $t$  at position  $\vec{r}$  and of velocity  $\vec{v}$  per unit volume per unit "velocity volume";  $\Sigma(|\vec{v}|)$  is the probability per unit path length for the occurrence of any type of scattering process to a neutron of speed  $|\vec{v}|$ .  $\sigma(\vec{v}, \vec{v}')$  is the probability per unit path length per unit velocity volume  $d\vec{v}'$  that a neutron of velocity  $\vec{v}$  result from a scattering or multiplication process suffered by a neutron of velocity  $\vec{v}'$ ;  $s$  the distance from the point  $r$  to the position of the scattering or multiplication process. The range of  $s$  is from zero to  $s_{max}$  at the boundary of the medium. If the medium is not homogeneous,  $\sigma(\vec{v}, \vec{v}')$  and  $\Sigma(|\vec{v}|)$  may also be functions of position.

Two approximations have been used to make the integral equation more tractable: The neutrons have been treated as monochromatic, and the scattering and multiplication as isotropic. Corrections for the errors introduced by these simplifications are discussed below. For monochromatic neutrons the magnitude of the velocity may be taken to be unity by suitable choice of the unit of time. For isotropic scattering and multiplication of monochromatic neutrons  $\Sigma(|\vec{v}|)$  and  $\sigma(\vec{v}, \vec{v}')$  are constants, and will be written as  $\Sigma$  and  $(1+f)\Sigma/4\pi$  respectively. Here  $\Sigma$  is the total cross section for scattering or multiplication,

$$\Sigma = \Sigma_s + \Sigma_m$$

$$f = \Sigma_m/\Sigma (\nu-1)$$

where  $\nu$  is the mean number of neutrons produced in a multiplication process;



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process.  $(1 + f)^0 / 4\pi$  is therefore the mean number of neutrons leaving the scene of a collision per unit solid angle. The use of these approximations depends on the choice of an appropriate average cross section and velocity. The methods of determining these appropriate averages will be discussed in section II. With these simplifications the integral equation (1) is best

written in terms of the total density,  $\rho(\vec{r}, t) = \int d\vec{v} \rho(\vec{r}, t, \vec{v})$ .

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$$\rho(\vec{r}, t) = \int \frac{d\vec{r}'}{|\vec{r}-\vec{r}'|^2} \frac{1 + f}{4\pi} \sigma e^{-\sigma|\vec{r}-\vec{r}'|} \rho(\vec{r}', t - |\vec{r}-\vec{r}'|) \quad (2)$$

The time dependent solutions of primary interest are those of the form  $\rho(\vec{r}, t) = \rho(\vec{r}) e^{\lambda t}$ , in particular the highest  $\lambda$  consistent with the geometry specified (corresponding to the positive definite eigenfunctions  $\rho(\vec{r})$ ). For such exponentially time dependent densities the integral equation takes the form,

$$\rho(\vec{r}) = \int \frac{d\vec{r}'}{|\vec{r}-\vec{r}'|^2} \frac{1 + f}{4\pi} \sigma e^{-(\sigma + \lambda)|\vec{r}-\vec{r}'|} \rho(\vec{r}') \quad (3)$$

As here written, equations 1 to 3 apply only to homogeneous media. If the body considered is of two or more parts for which the total cross sections are the same but different multiplication properties then equations (2) and (3) are correct as written if  $f$  is understood to be the appropriate function of position. If the total cross section also changes from one part of the body to another then the factor  $\sigma$  in the integrand must also be made space dependent and the exponential factor reexpressed to take account of the variation of  $\sigma$  along the path  $\vec{r}$  to  $\vec{r}'$ .

If there is only one medium, equation (3) permits a similarity transformation. Changing the scale of length so that  $\vec{r} = \lambda \vec{x}$  changes (3) into an equation in  $\rho(\vec{x})$  identical with (3) except for the replacement of the factor  $(1 + f)\sigma$  by  $(1 + f)\lambda\sigma$ ,  $(\sigma + \lambda)$  by  $\lambda(\sigma + \lambda)$  and the geometric specifications—radius, side, etc., — multiplied by a factor  $1/\lambda$ . Thus a solution of (3) for a specified size and value of  $f$ ,  $\sigma$ , and  $\lambda$  implies the existence of a solution for the same value of  $\sigma$  and for a new size,  $f$ , and  $\lambda$  such that the reciprocal radius (or side, etc.),  $(1 + f)$ , and  $(\sigma + \lambda)$  are all changed affecting same factor.

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It may always be taken to be unity by a suitable choice of the unit of length.

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**B. The Character of the Solution in the Interior.**

A differential equation which approximates to the requirements of the integral equation (3) in regions far removed from any boundary or interface of two different media may be found by taking  $\rho$  to be a solution of the wave equation  $(\Delta + k^2)\rho = 0$ . (More strictly by expressing  $\rho$ , as can always be done, in terms of such wave equation solutions. It is then seen that only one value of  $k$  can enter.) The integration on  $r'$  is then carried to infinity with constant  $f$  and  $\sigma$ .

As the general "wave function" (the term will be used throughout in the sense of a solution of the equation  $(\Delta + k^2)\rho = 0$ ) can be built up from plane wave solutions and the kernel of the integral equation is spherically symmetric and linear, it suffices to use any one such. If then

$$\begin{aligned}
 \rho_{ikr} &= 2\pi\sigma \frac{1+f}{4\pi} \int_{-1}^1 d\mu \int_0^\infty dr e^{-(\sigma+\delta)r} \rho_{ikr} \\
 1 &= \frac{\sigma(1+f)}{2} \int_0^\infty dr e^{-(\sigma+\delta)r} \int_{-1}^1 d\mu \rho_{ikr} \\
 &= \frac{\sigma(1+f)}{k} \int_0^\infty \frac{dr}{kr} e^{-(\sigma+\delta)r} \sin kr = \frac{\sigma(1+f)}{k} \tan^{-1} \frac{k}{\sigma+\delta} \quad (4)
 \end{aligned}$$

or for a hyperbolic wave function,  $\rho_{kx}$ ,

$$1 = \frac{\sigma(1+f)}{k} \tanh^{-1} \frac{k}{\sigma+\delta} \quad (4')$$

Expanding the  $\tan^{-1}$  to two terms gives an algebraic approximation to this relationship determining  $k/\sigma$  from  $f$  and  $\delta/\sigma$ .

$$\begin{aligned}
 1 &= \frac{\sigma(1+f)}{k} \left( \frac{k}{\sigma+\delta} - \frac{1}{3} \left( \frac{k}{\sigma+\delta} \right)^3 + \dots \right) \\
 1 &= \frac{1+f}{1+\delta/\sigma} \left( 1 - \frac{1}{3} \left( \frac{k}{\sigma+\delta} \right)^2 + \dots \right) \\
 \left( \frac{k}{\sigma+\delta} \right)^2 &= 3 \left( \frac{f - \delta/\sigma}{1+f} \right) \quad (5)
 \end{aligned}$$

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Evaluating  $k/\sigma'$  for the critical case ( $\beta = 0$ ) and for, say,  $f = \frac{1}{3}$ , by the use of equations (4) and (5) gives  $k/\sigma' = 1.45$  and 1.000 respectively. The two term expansion is thus not sufficiently accurate. (As is to be expected since in this range the power series is not convergent.)

Still another simple approximate equation is that of "elementary diffusion theory." Treating the flux of neutrons as in elementary kinetic theory gives:

$$-\frac{1}{3} \nabla^2 \phi + f \sigma' \phi = \beta \phi$$

$$(k/\sigma')^2 = 3(f + \beta/\sigma')$$
 (6)

which is equivalent to equation 5 for critical cases and small  $f$ ; for non-critical cases (6) gives a value of  $k$  which is equal to the  $k$  of (5) divided by the square root of  $1 + \beta/\sigma'$ .

### G. Boundary conditions for an approximate analytic solution.

The replacement of the integral equation (3) by the wave equation with its scale factor determined by equation (4) gives quite accurately the condition on the form of the neutron distribution in the deep interior of the body and a fair representation even close to the surface or interfaces, but it does not provide a boundary condition. If the wave equation is used to specify the form of the solution thruout the interior or the interiors of all the separate regions involved, the requirement that the wave equation solution satisfy the integral equation at the surface supplies a boundary condition. As the integral involved is difficult to evaluate, even for the simplest wave functions, it is convenient to approximate to the integral by treating the boundaries as plane and replacing the wave functions by the corresponding plane waves. Thus, for example, in the problem of the untamped (homogeneous) sphere the solution is  $(\sin kr) / r$ , with  $k$  determined by equation (4), and the radius

$$\begin{aligned} \sin ka &= 2\pi \int_0^a \frac{1+f}{4\pi r^2} \left[ \int_0^r dr e^{-(\sigma+\gamma)r} \right] \sin k(a-r) \\ 1 &= \frac{1}{2\pi a} (1+f) \int_0^a \left[ \int_0^r dr e^{-(\sigma+\gamma)r} \right] (\cos k'r - \cot ka \sin k'r) \\ &= \frac{1}{2\pi a} (1+f) \left\{ \frac{1}{k} \tan^{-1} \frac{k}{\sigma+\gamma} - \frac{1}{2k} \cot ka \ln \left( 1 + \frac{k^2}{(\sigma+\gamma)^2} \right) \right\} \\ \therefore \tan ka &= \frac{\sigma(1+f) \ln \left( 1 + \frac{k^2}{(\sigma+\gamma)^2} \right)}{2k} = \frac{-\ln \left( 1 + \frac{k^2}{(\sigma+\gamma)^2} \right)}{2 \tan^{-1} \left( \frac{k}{\sigma+\gamma} \right)} \quad (7) \end{aligned}$$

In the problem of the tamped sphere the body consists of a spherical core in which multiplication occurs, surrounded by a spherical shell of material (the tamper) for which  $\sigma$  may or may not have the same value as in the core and for which  $f = 0$ . Then in the core the solution has the form  $(\sin kr) / r$  and in the tamper  $(\sin (k'r-B)/r)$  or  $(\sinh (B-k'r)/r)$  as  $\gamma$  is negative or positive. The phase of the sin or sinh at the outer boundary of the tamper is determined by equation (7) or the corresponding condition for the sinh:

$$\begin{aligned} \tan (k'b-B) &= \frac{-\ln \left( 1 + \frac{k'^2}{(\sigma+\gamma)^2} \right)}{2 \tan^{-1} \left( \frac{k'}{\sigma+\gamma} \right)} \\ \tanh (B-k'b) &= \frac{-\ln \left( 1 - \frac{k'^2}{(\sigma+\gamma)^2} \right)}{2 \tanh^{-1} \left( \frac{k'}{\sigma+\gamma} \right)} \quad (7') \end{aligned}$$

where  $b$  is the radius of the outer boundary of the tamper.  $k'$  is determined by equation 4 or 4', using the tamper value of  $\sigma$ , an assumed  $\gamma$ , and  $f = 0$ . This, with a specified tamper thickness, determines the phase of the tamper solution at the inner surface. The phase of the core solution, hence the core radius, is then determined by an equation similar to (7) which equates the common value of the two solutions at the interface to the sum of the two contributions to the integral.

$$\frac{\cot ka \ln \left( 1 + \left( \frac{k}{\sigma - \gamma} \right)^2 \right)}{\tan^{-1} \frac{k}{\sigma + \gamma}} = \frac{\cot (k' a - B) \ln \left( 1 + \left( \frac{k}{\sigma + \gamma} \right)^2 \right)}{\tan^{-1} \frac{k'}{\sigma + \gamma}}$$

$$= \frac{\coth (B - k' a) \ln \left( 1 - \left( \frac{k'}{\sigma + \gamma} \right)^2 \right)}{\tanh^{-1} \frac{k'}{\sigma + \gamma}}$$

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 $\gamma > 0$

The errors of this analytic approximation method are confined to small regions around the boundaries. They are thus greatest for small untamped spheres and vanish with increasing core and tamper thickness.

The boundary condition consistent with the assumptions of the elementary diffusion theory is the continuity of the density and its derivative divided by  $\sigma$ . This requires the vanishing of  $\rho^2$  at the outer boundary which is at variance both with the analytic approximation and numerical results. The offset, the distance from the boundary to the zero of the analytic solution, is one half mean free path for a critical tamped sphere or for an infinite untamped sphere and approximately one half for finite size and  $\gamma^*$ . The elementary diffusion theory is therefore reasonably accurate only for radii very large compared with a half mean free path.

Some results of the three methods of calculations which are of interest are:

	anal.	radius numer.	el. diff.
$f = \frac{1}{3}, \gamma = 0, \text{ untamped}$	1.80	1.73	2.57
$f = \frac{1}{2}, \gamma = 0, \text{ tamper thickness } 2$	1.31	1.34	1.60
$f = \frac{1}{3}, \gamma = 0, \text{ infinite tamper}$	1.07	----	1.28

D. The exact solution of the integral equations.

Since the integral equation is linear and homogeneous a solution can be found by successive application of the integral operation to an assumed trial function. The assumed trial function will consist of a superposition of eigenfunctions of the equation. The fundamental mode corresponding to the highest eigenvalue, will predominate after a sufficient number of iterations.

\* In error; Cf. LA-8.

Since the fundamental is the only solution which is everywhere positive there is no danger of choosing a trial function which contains it only in small part. For a sphere, tamped or untamped, the integral equation (3), by doing the angular integrations, can be put in the form.

$$u(r) = r^{\sigma} \phi(r) = \int dr' \frac{1+f}{1+\gamma/\sigma} u(r') \left[ E(r-r') - E(r+r') \right]$$

Where  $E(X) = \int_x^{\infty} \frac{e^{-y}}{y} dy$

For a kernel of this type, consisting of the sum of two terms which for different  $r$  values differ only by a displacement in  $r'$ , the integration can be carried out numerically with comparative ease. This ease of integration permits the iteration to be continued until any desired accuracy is attained. By this means  $\gamma$  was determined for a considerable number of choices of  $f$  and the inner and outer radii. By comparison with these exact solutions the accuracy of various analytic approximations considered has been ascertained.

Work is in progress which it is hoped will lead to an exact analytic solution to the problem or at least to a better analytic approximation.

## Section II. The Evaluation of the Physical Constants

In problems in which the slowing of the neutrons or the inhomogeneity of the neutron spectrum is significant this inhomogeneity can be taken into account by treating the neutrons as separated into two or three phases, the slowing being represented by transitions from one phase to another. These problems have been treated by Serber using elementary diffusion theory. This same method can be applied to the integral treatment.

If the scattering of the neutrons cannot be treated as isotropic the integral equation (3) must be modified. There will still exist a unique wave function solution but the determination of  $k$  will depend on the details of the angular distribution. In the limit of small  $k$ , the elementary diffusion theory limit, the same relationship between  $k$  and  $\gamma$  will hold.  $\sigma$  is interpreted

as the transport cross-section  $(1 - \cos \phi) \sigma_t(\phi)$ .

If  $k$  is comparable with

unity equation (4) may be replaced by:

$$\frac{1 + \delta/\sigma_s}{1 + f} = \frac{\tan^{-1} k}{k} - \frac{\sigma_t}{k^2(\sigma_s + \delta)} \left( 1 - \frac{\tan^{-1} k}{k} \right)$$

$$1 - \frac{\sigma_t}{k^2(\sigma_s + \delta)} \quad 1 - \tan^{-1} \frac{k}{k}$$

where  $k = \frac{k}{\sigma_s - \delta}$  and  $\sigma_s$  and  $\sigma_t$ , are the first two Legendre coefficients in the scattering cross-section. Similar extended expressions can be used if the higher Legendre coefficients are significant. These equations are derived from the exact solution:

$$\sum_{n=0}^{\infty} \sigma_n \sum_n (P_n) = \frac{1}{\sigma_s + \delta - \frac{1}{k}} \sum_{n=0}^{\infty} \frac{\sigma_n P_n(k)}{2n+1} (1 + f \sigma_n)$$

where the  $n$ 's are the Legendre coefficients of the angular distribution of the neutrons.



The determination of the critical mass of a fissionable material depends on the rate of growth or decay of the neutron distribution in a non-critical amount of the material depends on the solution of an integral equation.

$$\rho(r) = \int \frac{dr'}{|r-r'|^2} \frac{1-f}{4\pi} \sigma_c - (\sigma_c - \sigma_f) |r-r'| \rho(r') \quad (a)$$

Here  $\rho(r)$  is the density of neutrons at the point  $r$  without regard for direction of motion.  $\sigma$  is the reciprocal mean free path for any type of collision, scattering, capture, or fission. It is here assumed that all of the scattering is isotropic and that all cross-sections are independent of velocity. The fact that the actual scattering is not isotropic can be taken into account by introducing for the scattering cross-section an appropriate average value. The nature of this averaging process is discussed in section II. Similarly it is to be assumed that all neutrons have an appropriate mean velocity. The above integral equation applies only to the dominant solution of the time-dependent integral equation, that solution which increases most rapidly or decreases most slowly in time, with the time dependence  $e^{\lambda t}$ .  $t$  is here measured in units such that the velocity is unity.  $1+f$  represents the multiplication of the neutrons per collision, thus for each neutron collision a mean number  $1+f$  neutrons emerge. The above equation is obtained by equating the neutron density at each point to the sum of the contributions to it from all other points, taking account of the attenuation due to scattering and the change in time of the scale of the distribution.

The simplest approach to the solution of the equation (a) is to use the approximation of elementary diffusion theory, the assumption that the neutron density changes very slightly within a mean free path and very slowly with time. With this approximation the integral equation is replaced by a differential equation of the form:

$$(\Delta + K^2)\rho = 0 \quad K^2 = 3(f - \frac{\lambda}{\tau}) \quad (b)$$

obtained from a continuity equation by the boundary condition that the neutron density is zero at the boundary.

condition consistent with this treatment is the assumption that at the outer boundary the neutron density vanishes and that at any interface of two types of material the density and flux is continuous.

With this approximation the critical radius can be found. For  $f = \frac{1}{2}$  which is consistent with present knowledge of the physical constants involved, the critical radius for a naked sphere is 2.57 mean free paths. So small a radius is not consistent with the assumption of a slowly varying neutron distribution. Therefore, more accurate methods of solution are required.

A better approximation to the integral equation is obtained by assuming that the neutron distribution is a wave function solution,  $e^{ikx}$  or  $e^{-ikx}$ , and evaluating  $k$  by substitution in the integral equation, (assuming the boundaries infinitely far from the region considered.) This gives for  $k$

$$\frac{1 + \delta/\sigma}{1 + f} = \frac{\tan^{-1} k/\sigma + \delta}{k/\sigma + \delta} \quad \text{or} \quad \frac{\tanh^{-1} k/\sigma + \delta}{k/\sigma + \delta} \quad \text{respectively.} \quad (c)$$

The value of  $k$  so determined gives very accurately the shape of the neutron distribution in the interior, holding good to within about a half a mean free path of the boundary. In the limit of small  $k$  the above expression reduces to

$$k^2 = 3 (1 + \delta/\sigma)^2 \frac{(f - \delta/\sigma)}{(1 + f)} \quad (d)$$

In the limit of small  $f$  and  $\delta$  this reduces to (b). While for large  $k$  both (d) and (b) are quite wrong, for small  $k$  (d) is more accurate than (b), particularly if  $f$  and  $\delta$  are appreciable.

With the interior behavior of the solution determined by (c) it is only necessary to find an appropriate boundary condition to have an analytic approximation to the solution. The boundary condition that has been used is the requirement that if the interior solution be continued to the surface it there satisfy the integral equation. This leads for a typical untarped sphere to a sine solution vanishing about one half mean free path beyond the boundary.

Since the integral equation (a) is linear and homogeneous an exact

solution can be found by iteration. A trial function is assumed and the integral operation applied repeatedly until the successive approximations to  $\rho$  differ only by a constant factor. The integral operator for a sphere can be put into a numerically convenient form so that the integration can be carried out with considerable accuracy. This process has been carried out roughly for many cases and conscientiously for a few cases and proves that the analytic approximation previously discussed is reliable for both tamped and untamped spheres to about .01 in  $\delta/\sigma$ .

The appended curves give the results of this analysis.

In any particular case of interest for a tamped or untamped sphere  $\delta$  can be determined with great accuracy by numerical integration using the analytic approximation as a first trial function.

It has proved possible to find exact analytic solutions to the integral equation for the untamped or infinitely tamped half-infinite slab. It is hoped that the same methods may lead to exact solutions for the spherical problems.

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